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Representing Model Inadequacy in Combustion Kinetics REBECCA E. MORRISON, ROBERT D. MOSER, The University of Texas at Austin — An accurate description of the chemical processes involved in the oxidation of hydrocarbons may include hundreds of reactions and thirty or more chemical species. Kinetics models of these chemical mechanisms are often embedded in a fluid dynamics solver to represent combustion. Because the computational cost of such detailed mechanisms is so high, it is common practice to use drastically reduced mechanisms. But, this introduces modeling errors which may render the model inadequate. In this talk, we present a formulation of the model inadequacy in reduced models of hydrogen combustion. Our goal is to account for the discrepancy between the high-fidelity model and its reduced version by incorporating an additive, linear, probabilistic inadequacy model. In effect, it is a random matrix, whose entries are characterized by probability distributions and which displays interesting properties due to conservation constraints. The distributions are calibrated via Bayesian inference using a hierarchical modeling scheme and high-dimensional MCMC. We apply this technique to a stand-alone reaction and also incorporate it within a one-dimensional laminar flame problem.

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